

# Stochastic Optimization for Optimal Design and Operation of Quantum Devices, Algorithms, and Simulations

Jeffrey Larson and Stefan Wild

Mathematics and Computer Science Division  
Argonne National Laboratory

November 20, 2017

# QC Challenges & Opportunities → Optimization

*Key challenges for design and operation:*

- ▶ Determining operational parameters for extended entanglement
- ▶ Quantum chip design
- ▶ Inherent stochasticity and noisy operation
- ▶ Algorithm design for near-term hybrid devices
- ▶ Simulation of future devices

## Leverage Argonne strengths in computing & optimization

$$\underset{x \in \mathcal{D}}{\text{minimize}} \mathbb{E}_{\xi} [f(x; S(x; \xi))]$$

- ▶ Objective  $f$  depends on simulation (or physical system) output  $S(x)$
- ▶ Derivatives of  $S$  may not be available
- ▶ Constraints defining  $\mathcal{D}$  may or may not depend on  $S$
- ▶ Dimension  $n$  is relatively small

**Need specialized methods that exploit problem structure/knowledge**



# Initial Work: ASCR-Funded Quantum Algorithm Team

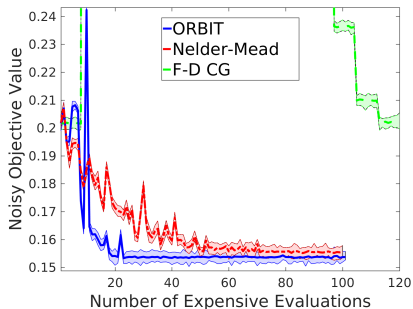


UCBerkeley 8-qubit device  
>  $7^2$ -qubit DOE device  
expected in 2018

LBNL+ANL+UCB+Harvard project

- ▶ novel quantum chemistry algorithms
- ▶ compilation, scheduling tools
- ▶ optimization, linear algebra

to model dynamical processes in chemistry  
(e.g., time dynamics quantum simulations)



Argonne's ORBIT for optimal state preparation of  
variational quantum eigensolver